ADVANCEMENTS IN FUEL SPRAY AND COMBUSTION MODELING WITH HIGH-PERFORMANCE COMPUTING (HPC) RESOURCES

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Project ID # ACS075

OVERVIEW

Timeline

Project start: FY 2012
Part of 2017 VTO Lab Call

Budget

FY 16: $ 970 K (2 combined tasks)
FY 17: $ 820 K (2 combined tasks)
FY 18: $ 600 K *(2 combined tasks)

* Funds for FY18 reflect a reduced spending rate

Partners

Argonne National Laboratory
- Leadership Computing Facility (ALCF)
- Advanced Photon Source

Convergent Science Inc. (CSI) } CRADA
Cummins Engine Company
Automotive OEMs (GM, Ford, FCA)
Lawrence Livermore National Laboratory
Sandia National Laboratory
Esgee Technologies

Small Business Programs (SBIR, SBV)
Advanced Engine Combustion (AEC)
University of Connecticut
University of Perugia (Italy)
Michigan Technological University
North Carolina State University
Several more Universities involved in FOAs

Barriers

- ❑ "Inadequate understanding of the stochastics of fuel injection"
- ❑ "Limited understanding of analysis tools for advanced ignition systems"
- ❑ "Improving the predictive nature of spray and combustion models"
- ❑ "Incorporating more detailed chemical kinetics into fluid dynamics simulations"
- ❑ "Development of HPC tools to provide unique insights into the fuel injection, ignition, and combustion processes"

OBJECTIVES AND APPROACH

In general Engine simulations involve:

- Unresolved Nozzle flow
- Simplified combustion models
- Coarse mesh => grid-dependence
- Poor load-balancing algorithms
- Simplified turbulence models

Extensive tuning to match experimental data

High-Fidelity Approach:

- Fuel spray and nozzle-flow models
- Detailed chemistry based combustion models
- Fine mesh => grid-convergence
- Improved load-balancing algorithms with METIS
- High-fidelity turbulence models: LES based

- Exascale Computing

Towards Predictive Simulation of the Internal Combustion Engine

- ❖ Develop reliable engine modeling capability with fewer tuning constants
- ❖ Sub-models published in open-literature and available to the industry through software packages
- ❖ Develop “engineering best practices” for industry to use these high-fidelity models

RELEVANCE – ACCURACY, SPEED, AND AVAILABILITY*

- **Nozzle flow and Spray research**
  - Cavitation erosion continues to be a concern, and in general the modeling tools are not predictive.
  - X-ray measurements at Argonne can now provide real injector geometry with ~1 µm resolution.
  - Approach to fully coupled nozzle flow and spray simulations developed and published.
- **Advanced Ignition Research**
  - Relevant to SI as well as mixed-mode combustion. Challenging operation, requires predictive SI models.
  - No models are available for non-conventional ignition systems [Low-temperature plasma (LTP)].
  - LESI model copyrighted and available. LTP ignition models are being developed for commercial codes.
- **Combustion modeling using detailed chemistry**
  - Tabulated Flame Model (TFM) can enable the use of full chemistry (without mechanism reduction) for compression ignition engine simulations. However, table sizes can be very large.
  - TFM is currently available through UDFs that can be ported to any academic or commercial code.
- **High-Performance Computing (HPC)**
  - Ensuring that the computational tools can scale in the next-generation exascale platforms such as Aurora (First exascale supercomputer available at Argonne in 2021)
  - Ported Converge (commercial) and Nek5000 (open-source) codes on Theta (similar hardware as Aurora) for scaling studies on engine simulations

Mira: 10 petaflops

Aurora: Exascale

* DOE-VTO workshop to identify roadmap for CFD organized by Leo Breton in 2014

SIMULATION APPROACH: SUB-MODEL DEVELOPMENT

Modeling Tool	CONVERGE
Smallest and largest characteristic grid size(s)	**Finest grid size simulations:** **2.5 µm for nozzle flow (35 million cells)** **~30 µm for GDI and diesel Sprays (20 million cells)**
Turbulence-chemistry interaction (TCI) model	**Tabulated Flamelet model (TFM)** **Homogeneous Reactor based model (HR)**
Turbulence model(s)	LES: Dynamic Structure sub-grid scale model ✓ Extensive nozzle flow and GDI spray simulations
In-nozzle Flow	**New Criteria Proposed for Cavitation Erosion** **Homogeneous Relaxation Model (HRM)** ✓ Diesel and gasoline injectors ✓ Extended for multi-component fuels
Spray models	Volume of Fluids (VOF) approach for phase-tracking **Coupled Eulerian-Lagrangian Spray Atomization (ELSA) Model** **One-way coupling approach**
Ignition Modeling	**Lagrangian-Eulerian Spark-Ignition (LESI) Model** **Mixed (Energy and Species) deposition model for LTP ignition**

Extensive validation against data from several collaborators at Argonne (C. Powell), Sandia (L. Pickett, I. Ekoto, C.J. Mueller), Academia (S.Y. Lee, J. Naber)

Argonne NATIONAL LABORATORY

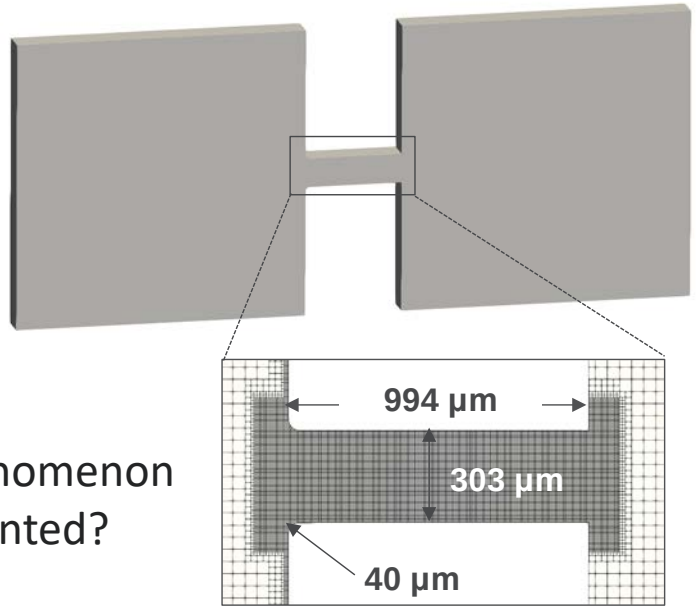
MILESTONES FOR FY 18

- Nozzle flow and Spray Research (CRADA with Cummins and CSI)
  - Integrate flash-boiling approach with advanced turbulence model and validate against experimental data {75% complete}
  - Develop in-nozzle cavitation erosion model for diesel injectors and validate against optical data available in literature and new data from APS {50% complete}
- Ignition and Combustion Modeling
  - Develop and implement comprehensive ignition model to simulate ignition from thermal and non-thermal plasmas {50% complete}
  - Perform extensive RANS and LES calculations with detailed and reduced 5-component diesel surrogate (against optical engine data from Sandia) to demonstrate the run-time vs. accuracy trade-off of turbulence and detailed kinetic models {75% Complete}
- High-Performance Computing
  - Import CONVERGE code on new architecture (theta) for the upcoming supercomputer Aurora and identify scaling bottlenecks {10% complete}

All the newly developed models and key findings are published in journal papers and peer-reviewed conference proceedings so that academia, OEMs, and other software vendors can benefit from our work. Several OEMs and software vendors have engaged with us through the VERIFI program

APPROACH: CAVITATION EROSION MODELING

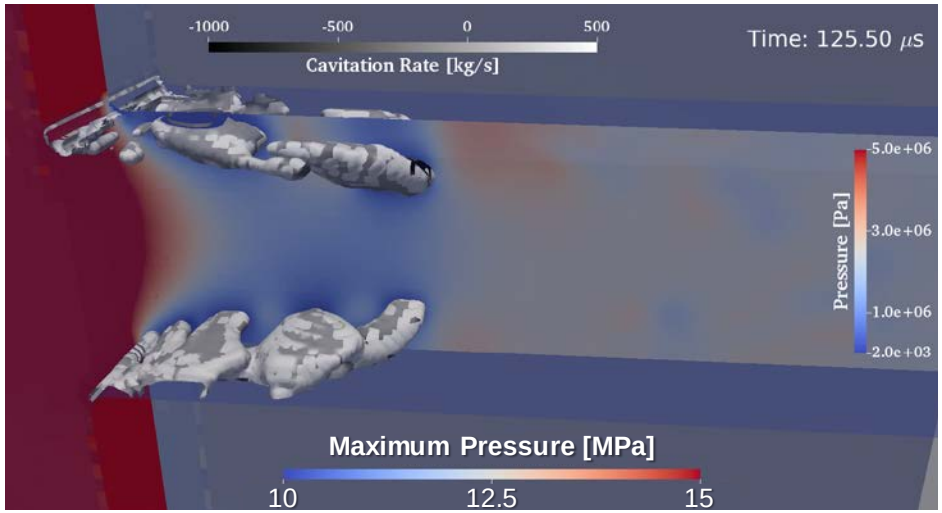
- Efficient indications of cavitation erosion are needed to identify critical flow conditions and locations.
- Rapid vapor cloud collapse produces a shock wave, which can cause impact stresses in excess of the material yield strength on neighboring surfaces.
- Tracking the maximum pressure can allow for efficient identification of single impact events.
- How can cavitation erosion, as a fatigue-driven phenomenon resulting from multiple impacts, be efficiently represented?



- PREVERO channel "K" geometry (Skoda et al., WIMRC 3rd Int. Cavitation Forum, 2011) modeled to study cavitation shedding and critical cloud collapse events.

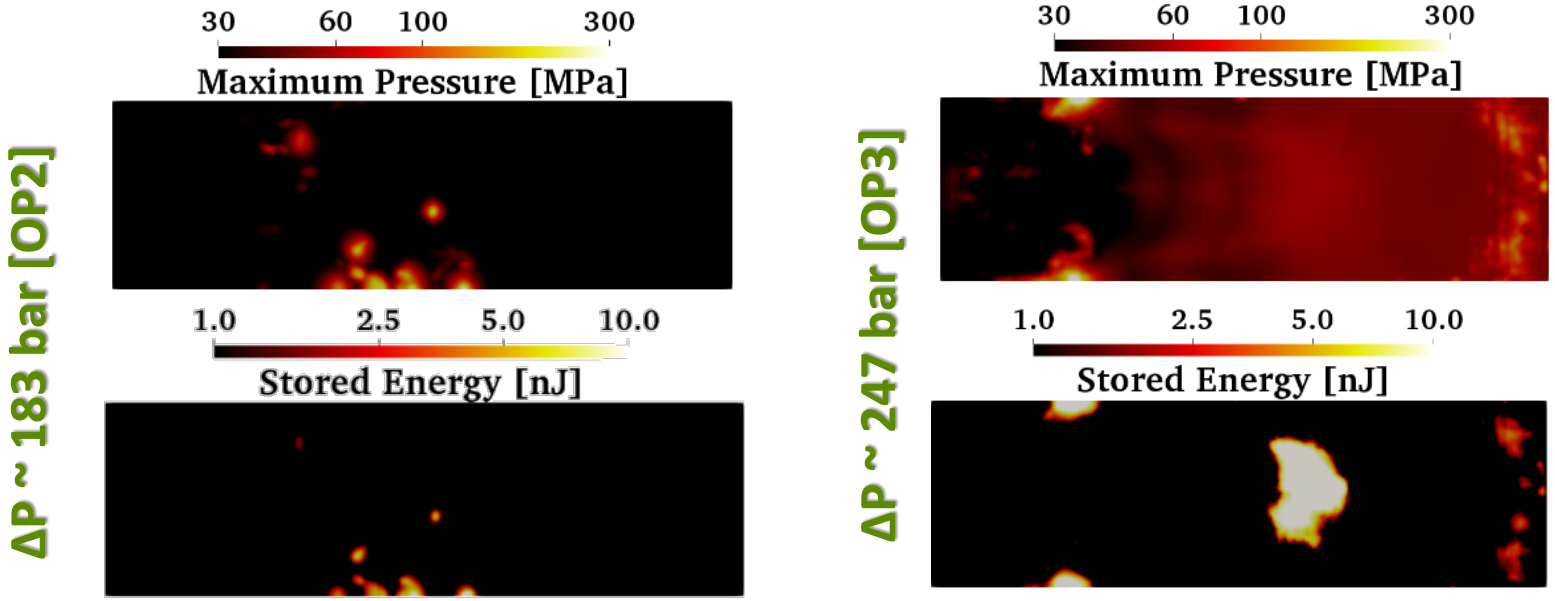
$$E_{stored}(N) = \sum_{i=1}^{N} \frac{\mathcal{A}}{\rho_l c_l} \int_0^{\tau} p^2(t)dt$$

p is predicted local pressure, density ρ_l and speed of sound c_l, and acts on the surface of area $\mathcal{A}$ over a duration of time τ



ACCOMPLISHMENT: FLOW AND CAVITATION LOCATION FAIRLY WELL PREDICTED

- Onset of choked flow condition at ~200 bar is well captured along with the mass flow rate* at all ΔP.
- Because the impact pressures at these locations are less than the ultimate stress of aluminum of 300 MPa, these high energy impacts are not likely to result in material rupture.
- Comparison of the predicted stored energy distributions for the OP2 condition and at the channel exit for the OP3 condition provides a qualitative assessment of relative incubation period before material rupture.
- The larger average stored energy for the OP2 condition in comparison to the OP3 condition suggests that the incubation period would be shorter under the OP2 condition. This result is consistent with the experimental findings*, where the incubation period for the OP3 condition was found to be relatively longer.
- These findings using the newly developed cavitation erosion metric highlight its utility in quantifying both the energy of single impact events, as well as the influence of repeated impacts on the incubation period before material rupture.

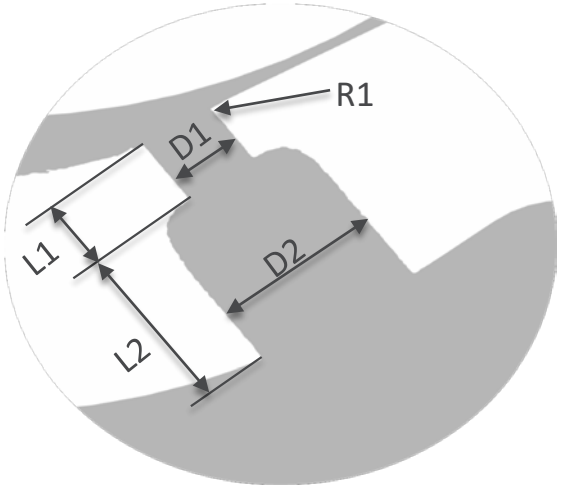


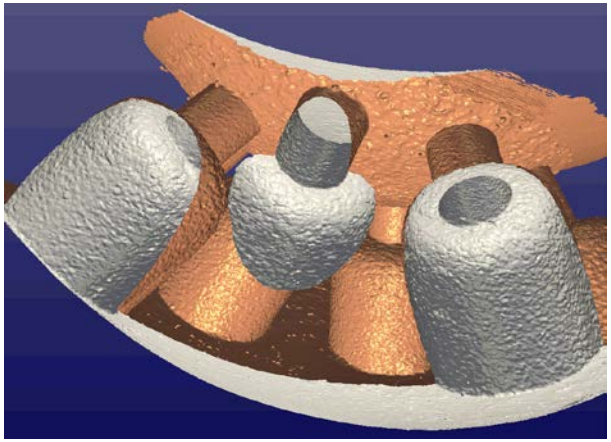
* Skoda et al., WIMRC 3rd Int. Cavitation Forum, 2011.

ACCOMPLISHMENT: REAL VS. NOMINAL GEOMETRY SIMULATIONS

- Micron-level high resolution real geometry of ECN Spray G injector, by X-Ray CT imaging at 7-BM beamline of APS at Argonne.
- Geometric features show considerable differences between measured values and nominal values.

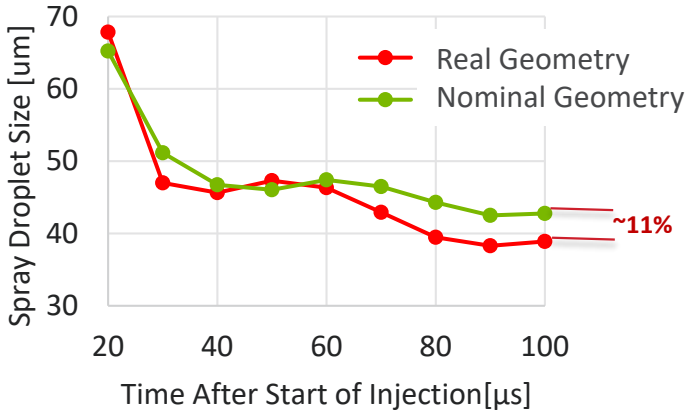
Geometric feature		Real	Nominal
Hole diameter	D1 [µm]	175	165
Hole length	L1 [µm]	150	170
Hole length/diameter ratio	L1/D1	0.86	1.03
Hole inlet corner radius	R1 [µm]	4.93	0
Counterbore diameter	D2 [µm]	394	388
Counterbore length	L2 [µm]	402	470

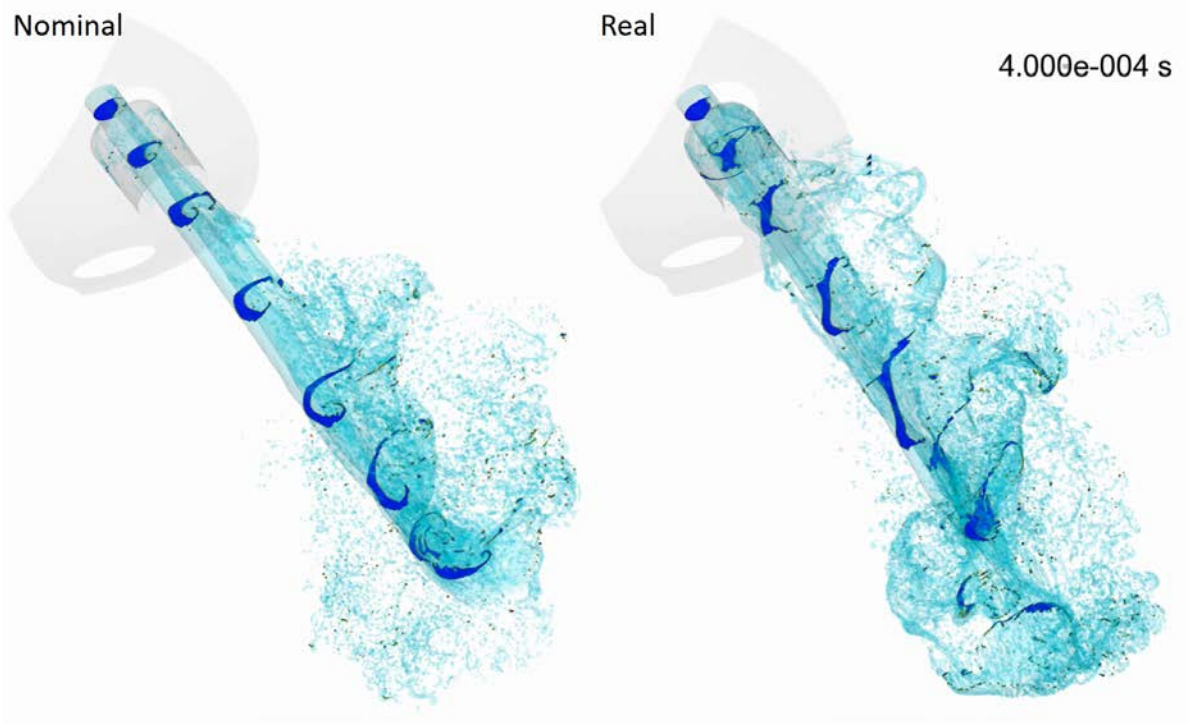




ACCOMPLISHMENT: REAL VS. NOMINAL GEOMETRY EFFECTS

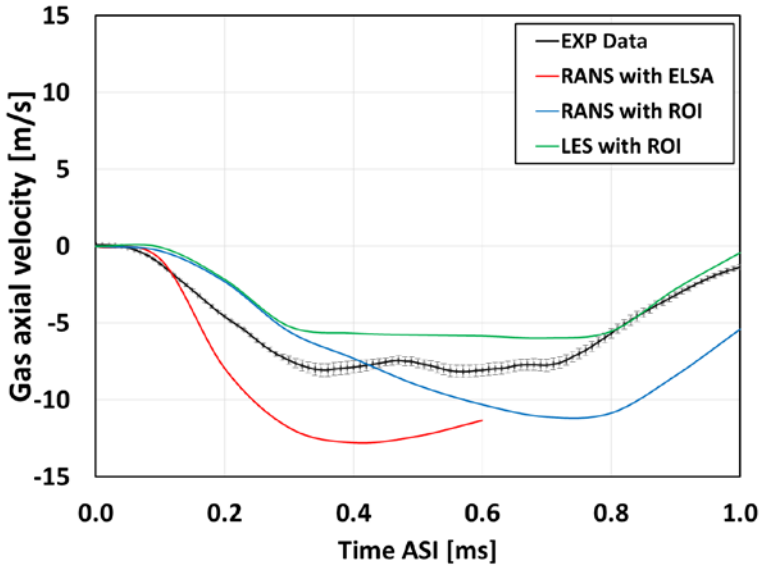
- First demonstration of real geometry effects on nozzle flow and sprays for GDI.
- 2.5 µm min. resolution, peak cell count of ~30 million, 10 days on 160 cores for about 0.1 ms calculation of needle opening.
- **More filled counter-bore, faster breakup of jet into ligaments and parcels, smaller SMDs with the real geometry.**

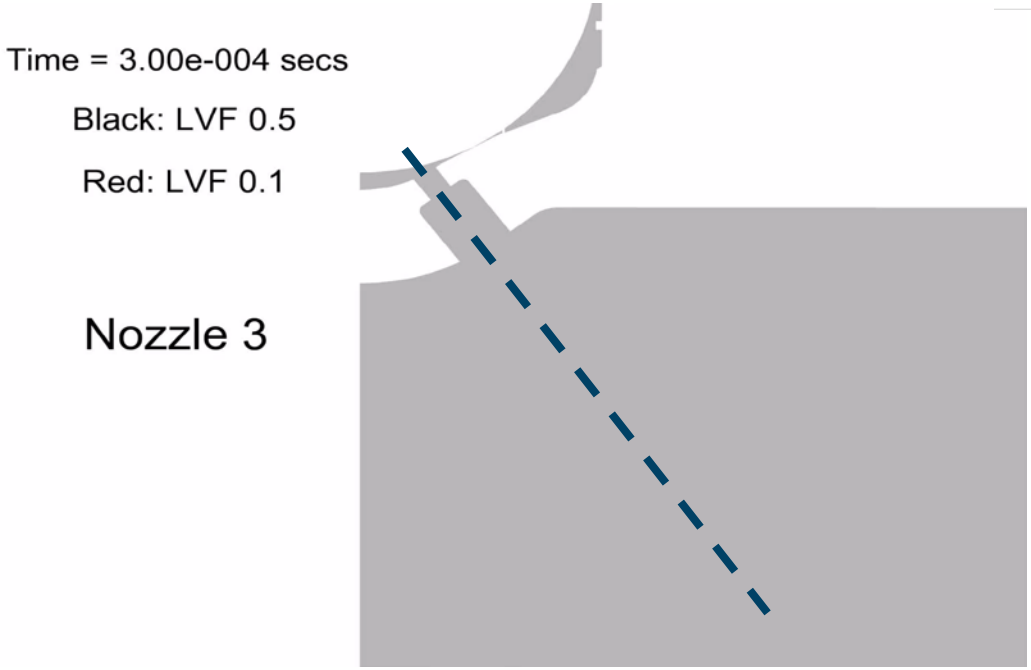




ACCOMPLISHMENT: MULTI-HOLE GDI SIMULATED WITH FULLY COUPLE ELSA MODEL WITH MOVING NEEDLE

- Further development of Eulerian Lagrangian Spray Atomization (ELSA) model from the AMR2017.
- First application on multi-hole injectors.
- Additional transport equation for ELSA implemented within the mixture multiphase modeling framework and tested with both URANS & LES.
- Moving needle Eulerian GDI calculations coupled with downstream automatic transition to Lagrangian parcels; 0.5 mm base grid; ~8 million cells; 15 µm inside the nozzle; 125 µm in spray region; 128 processors, 1 ms in 20 days.

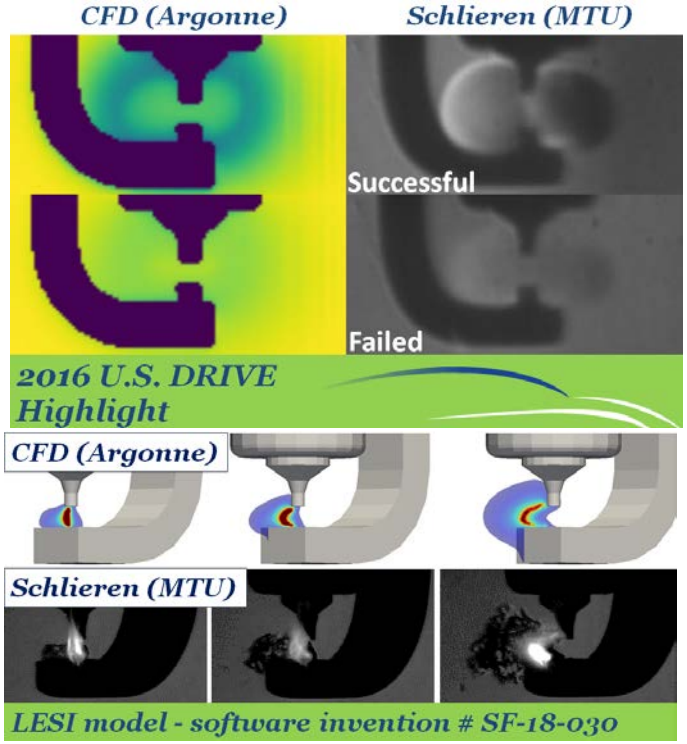


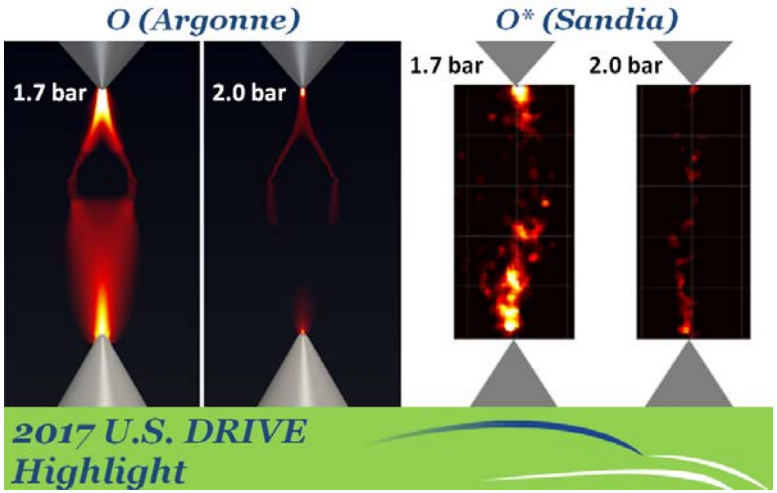


- Spray penetration and gas phase axial velocity (from Sandia experiments) are fairly well predicted using ELSA.
- ELSA allows for predictive simulations of spray penetration and liquid-gas coupling without the need for the typical inputs required by the Rate of Injection approach.
- ELSA needs further investigation, e.g. with respect to transition criteria (not shown here).

APPROACH: IGNITION MODELING

- Realistic source features and heat transfer calculations make SI models accurate at challenging operation (e.g. predicting misfires).
- Our hybrid LE approach combines the accuracy of the Eulerian deposition with the Lagrangian approach to resolve the evolution of the ignition source during the spark process **[Lagrangian Eulerian Spark Ignition (*LESI) model, software invention #SF-18-030*]**.
- Similar ignition mechanism (thermal energy deposition) can be used for other ignition technologies (i.e., laser).





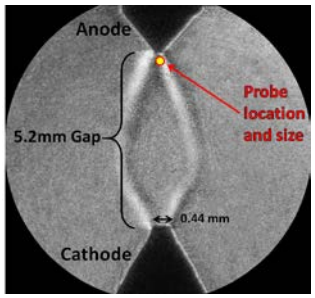
- More complex approach is needed for Low-Temperature Plasma (LTP) ignition (streamers, corona discharge, etc.).
- Dedicated non-equilibrium plasma solvers deliver proper understanding of the LTP thermal and chemical properties.
- The key question is how the combined chemical species and heat impact ignition.

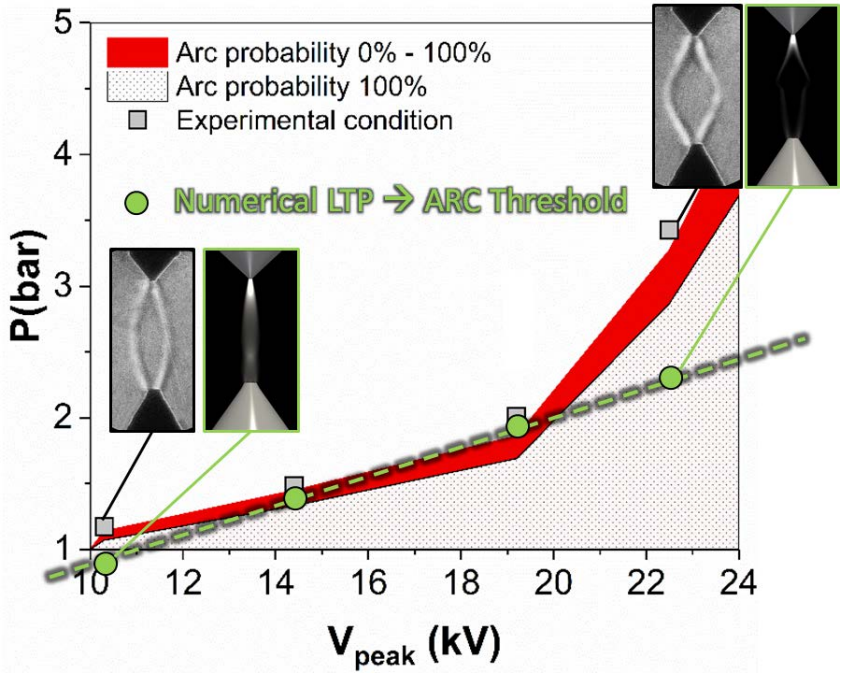
Our modeling progress was included in the *2016* and *2017 U.S. DRIVE Highlights of Technical Accomplishments*

ACCOMPLISHMENT: LTP MODELING VALIDATED AGAINST EXPERIMENTS

Improved numerical (ANL) and experimental (SNL) procedures delivered close agreement in terms of LTP thermal/chemical properties

- **SNL:** Better control of gas composition and electrode geometry
- **ANL**: Evaluation of initial conditions and model tuning ($E_{\text{cross section}}$)
- Quantitative comparison at same location (near the anode)





- LTP (glow) → ARC (spark) transition region quantitatively captured by simulations
- Disagreement persist at low/high voltage (simulations deliver consistent linear trends)
- Streamer appearance (increased branching at higher pressure) remains consistent

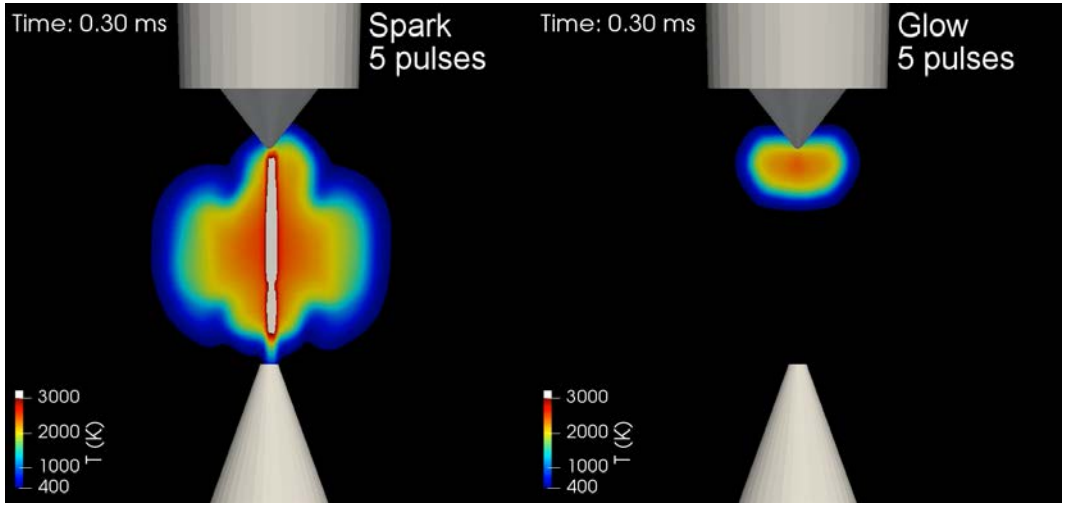
	SIMULATIONS		EXPERIMENTS	
	O (#/m³)	Temp (K)	O (#/m³)	Temp (K)
14kV - 1.5bar	0.9E+24	770	2.0E+24	847
19kV - 2.0bar	1.8E+24	938	2.3E+24	1237

- Very good (quantitative) agreement at same conditions (intermediate points)
- Timescales are different (ηs versus μs). VT relaxation will increase Temparature

Experimental data/images from Isaac Ekoto (ACS006)

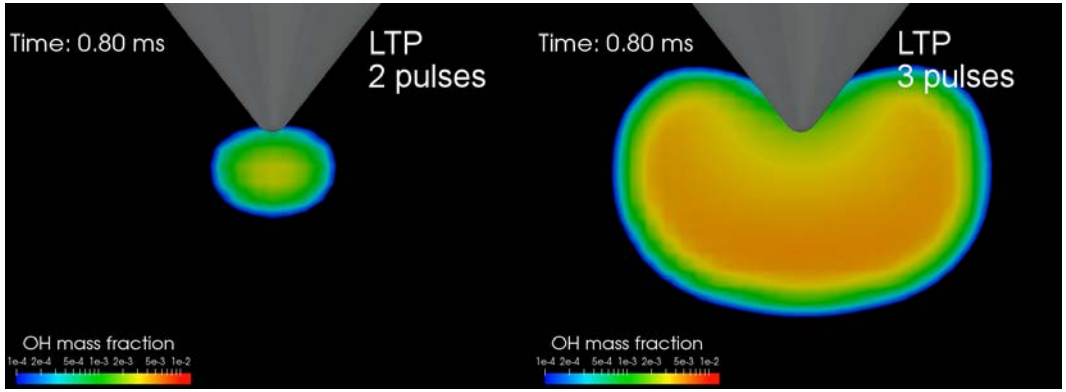
ACCOMPLISHMENT: LTP IGNITION SIMULATED WITH REALISTIC ENERGY/SPECIES DEPOSITION

- **Glow (LTP) Deposition:** Thermal energy and active species (O) resulting from LTP simulation (VIZGLOW) deposited at each pulse in the CFD flow simulation (CONVERGE).
- **Spark Deposition:** Total thermal energy measured in the experiments (Sandia) deposited.



- 5 pulses – 10kHz (0.1 ms dwell time)
- P = 1.5 bar, T = 343 K, ϕ= 1.0
- CONVERGE, RANS k-ε modeling
- SAGE, C_8H_{18} 110 species, 488 reactions
- **O deposition in the glow discharge triggers fuel chemistry and locally increases Temperature (still much lower than for the spark discharge)**

- LTP deposition quantities are critical, in particular the chemical component (O).
- **<u>Minimum concentration of radicals (i.e. minimum #pulses) is required to start reactions.</u>**
- Single-spark event ignites the mixture, several pulses might be needed for LTP ignition depending on the conditions.



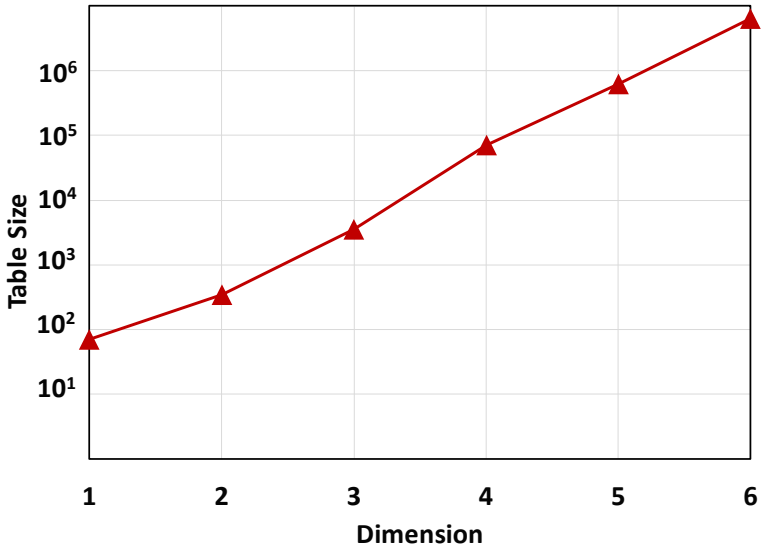
APPROACH: USE OF DEEP NEURAL NETWORKS FOR FLAMELET TABULATION WITHIN TFM* FRAMEWORK

- AMR2017 talk highlighted the development of the Tabulated Flamelet Model (TFM) that does not require mechanism reduction and allows for calculations with full chemistry [Software Invention # SF-16-159]. Some challenges were noted:
  - Table size increases exponentially with dimensions
  - Higher dimensional tables required for higher fidelity
  - Memory and retrieval costs increase exponentially
  - Modern architectures have lower memory per core

Multidimensional chemistry tabulation

Flamelet Equation: $$\rho \frac{\partial Y_i}{\partial t} = \rho \frac{\chi}{2} \frac{\partial^2 Y_i}{\partial Z^2} + \dot{\omega}_i$$

$$Y_i \rightarrow Y\left(\chi, t, \widetilde{Z''^2}, \widetilde{Z}\right)$$

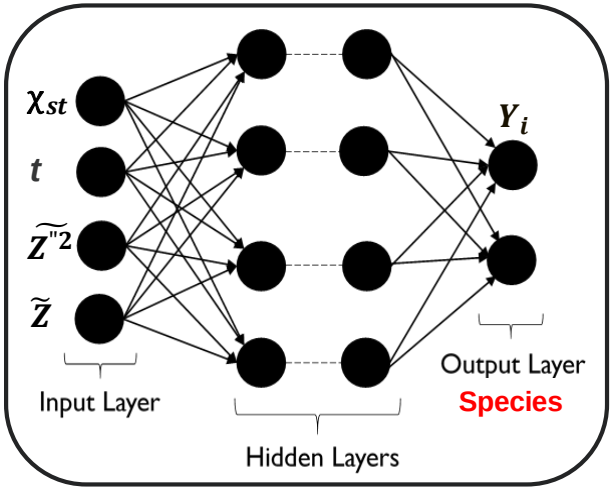


- Salient features: Incorporate Artificial Neural Networks (ANN) for tabulation
  Use LSODES solvers to implement 3000+ species detailed mechanisms for HC fuels
- Advantage: Significant reduction in memory footprint and computational cost.
- Manifold/application independent ANN formulation.
- Address the “curse of dimensionality” in tabulated models.

ACCOMPLISHMENT: ANN IMPLEMENTATION & VALIDATION

ANN algorithm

Use multidimensional flamelet manifold to train a Deep Neural Network

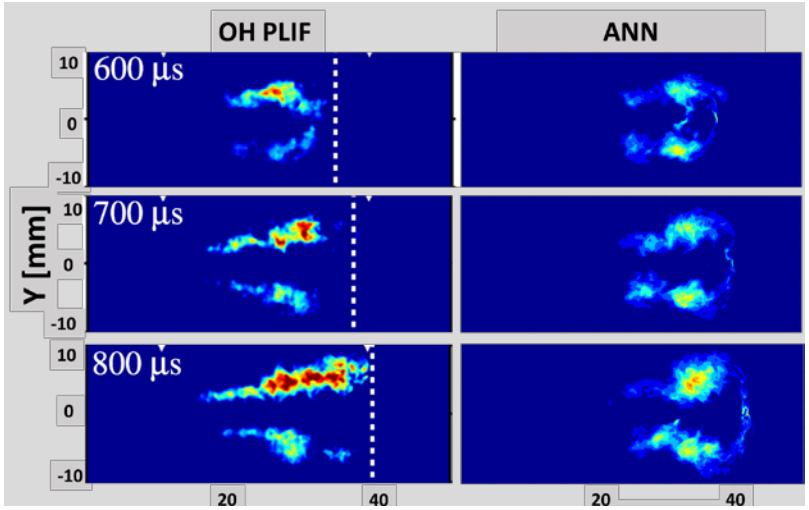


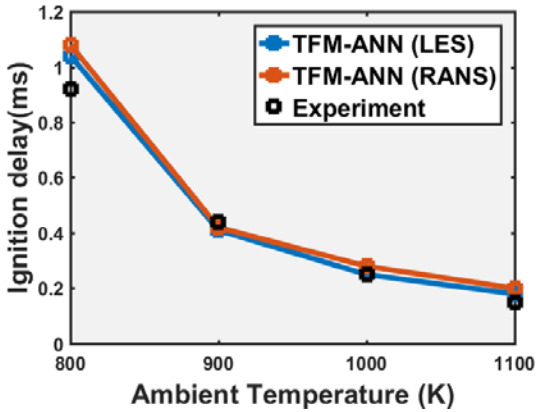
ANN features

- Novel bifurcation algorithms for multi-dimensional manifolds. Automated bifurcation of species.
- **1 GB flamelet table can be replaced by 85 KB ANN**
- Elimination of multi-dimensional interpolation

Validation: ECN Spray A data from Sandia

- LES with 22 million cells and 60 µm grid
- 103 species n-dodecane mechanism
- Ambient temperature range: 800 K – 1100 K
- Same ANN algorithm used over the entire range
- 4D flamelet table Y_i - $(\chi, t, \widetilde{Z''^2}, \tilde{Z})$





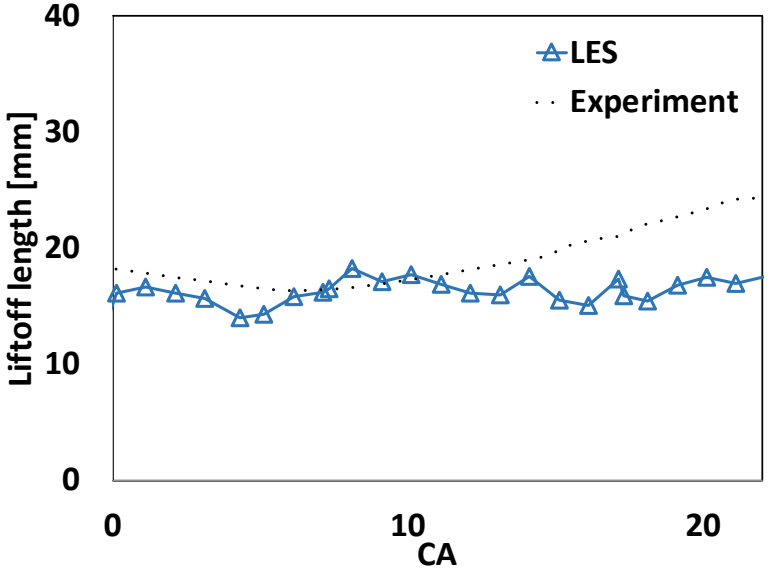
Ignition delay and flame lift-off length (LOL) along with the flame structure is well captured!

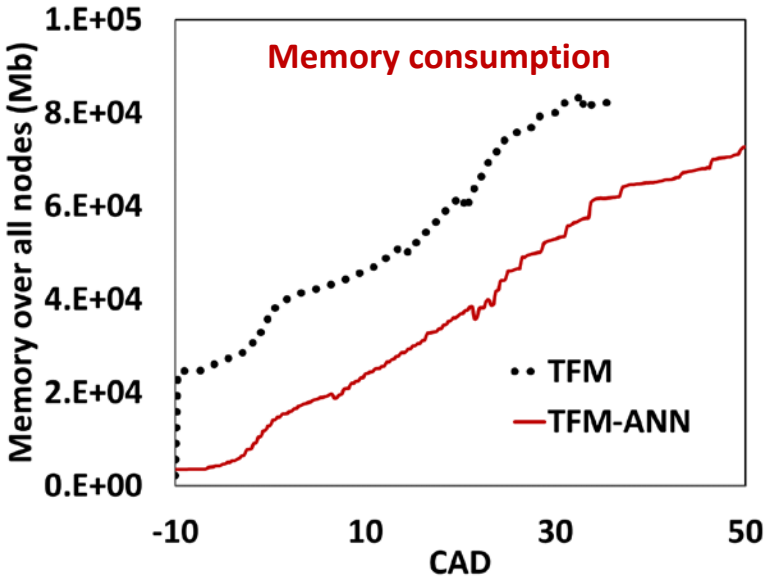
ACCOMPLISHMENT: VALIDATION WITH ENGINE DATA

Experimental data: Mueller's Optical Engine @ Sandia National Lab.

Simulation Details:

- Open cycle engine simulation with LES.
- Min. cell size: 90 µm grid; 25 million cells.
- Fuel: Methyl Decanoate ($C_{11}H_{22}O_2$)
- Full mechanism without reduction: 3299 species, 10804 reactions
- 5D flamelet table Y_i - $(P, \chi, t, \widetilde{Z''^2}, \tilde{Z})$.
- Simulation time: 160 Hours on 480 processors.





- ANN is able to capture the ignition delay and flame liftoff across different conditions.
- Accurately captures the onset & cool flame regions.

Advantages of ANN

- Lower memory footprint.
- **40 %** reduction in CPU costs.
- Higher savings for higher dimensional manifolds.
- Can be used with any tabulation methodology.

COLLABORATIONS

Argonne National Laboratory

- **Engine and Emissions Group: (Provide data for model validation)**
- **Leadership Computing Facility (Improving Scalability of CONVERGE, HPC resources)**
- **Advanced Photon Source: (Nozzle flow and Spray Data)**

Convergent Science Inc. (Algorithm and code development in CONVERGE)

Esgee Technologies Inc. (VIZGLOW code development and scalability testing)

Cummins (Provide experimental data, alpha testing of new models)

GM R&D (In-nozzle flow and spray simulations for GDI injectors)

Sandia National Laboratory (Provide experimental data on several projects)

Lawrence Livermore National Laboratory (Mechanism development)

University of Connecticut (Mechanism Reduction)

Michigan Technological University (Provide experimental data on ignition)

University of Perugia (In-nozzle Flow Simulations)

North Caroline State University (Turbulent Combustion Modeling with ANN)

Presentations at Advanced Engine Combustion (AEC) Working group

Engine Combustion Network Participation and Data Contribution

***Simulation Toolkit Team* in "Co-Optima" is leveraging our developments**

Three University FOAs are leveraging our developments

COLLABORATIONS THROUGH VERIFI

- Based on the capabilities developed under this program, we have established the Virtual Engine Research Institute and Fuels Initiative (VERIFI)
- VERIFI is designed to provide HPC solution for industrial problems of interest using either clusters of leadership class supercomputer such as Mira
- > 70 attendees for the 3rd workshop from light and heavy duty engine OEMS, software vendors, oil and energy companies, and Supercomputing solutions companies

FY 17 & 18

GE, aramco, Small Business Vouchers Pilot U.S. DEPARTMENT OF ENERGY, CONVERGENT SCIENCE, HPC 4 MANUFACTURING, U.S. DEPARTMENT OF ENERGY Energy Efficiency & Renewable Energy ADVANCED MANUFACTURING OFFICE, Ford, CAT, arpa·e, achatesPOWER, DELPHI

3rd workshop in November 2017

Understanding and Predicting Cyclic Variability in Engines

RESPONSE TO PREVIOUS YEAR REVIEWER COMMENTS

Overall the reviewers were positive about the progress of both the projects

Explain the novelty of the cavitation work and compare it with state-of-the-art.

The cavitation model is based on HRM and has been in existence for many years. We are adding additional details about the needle motion and wobble, real geometry effects, and a new erosion model to assess the effect of cavitation on material erosion.

Would like to see that the earlier work on wobble, reduced mechanisms for diesel surrogates, etc. are being used.

The in-nozzle flow work is being used in Cummins. The validated reduced mechanisms are used in ECN. An example of the use of needle wobble is also shown in the summary slide.

Project should not result in unfair subsidies for any specific commercial partner and does not create such an appearance now, or in the future.

As mentioned earlier as well, we publish all our findings in peer-reviewed articles. Other software vendors have also approached us to learn more about work. The use of a particular code as a demonstration platform for our models is driven by the OEM recommendations.

Would the authors be able to apply these improvements to selective engine test cases to assess and provide significant improvements can be made in the context of emissions and fuel economy?

The application of these models for engine simulations is currently being done within the Co-optima project and will be shown as part of three different presentations (FT053, FT054, FT055) for three different engine platforms.

…non-equilibrium plasma modeling that requires expensive chemistry could use some of the advanced solvers from project ACS012 or ACS076...the PI may need to collaborate with the LLNL algorithm investigators…

It is our plan too, but, first we need to evaluate the size of chemistry that needs to be resolved to properly simulate an LTP ignition. Collaboration with LLNL will be fruitful.

...questioned whether the proposed work in FY 2018 for cyclic variability requires LES. If yes, that can add significant computational cost to the already expensive chemistry for plasma modeling…

LES simulations can be carried out today at increasing mesh resolutions by leveraging large clusters and supercomputers. At this stage, switching from RANS to LES does not look like a challenging task.

…questioned if the proposed work will have an impact in removing barriers to high-dilution engines…

Our goal is to provide the modeling tools that can support this evaluation rather than making the evaluation itself. We are continuously required to provide more predictive models for each of the physics discussed here.

REMAINING CHALLENGES AND BARRIERS

- Cavitation Erosion: Extremely disparate time scales between cavitation and material fatigue leading to erosion. Collaborating with material scientists may provide insight into the appropriate coupling between CFD predictions and material behavior.
- Real Geometry: Computations with real geometry are extremely memory intensive and time-consuming regardless of the computational tool being used.
- Chemistry size:
  - LTP ignition requires plasma species (excited molecules and atoms, ions, electrons) and additional reactions (relaxation, dissociation, ionization) in addition to fuel chemistry. Size of mechanism can dramatically increase. Need to highlight/define important chemical pathways and work with fast chemistry solvers (LLNL projects).
  - Uncertainty in chemical kinetic mechanisms need to be documented.
- Computational resources: Coupling large chemistry with LES turbulence modeling can increase the computational resources needed to perform these simulations.
- High-fidelity experimental engine data: We need dedicated experiments to validate some of our models and at times this dataset is not available and needs to be generated. Also, we need uncertainties in measured data. Simulations do not account for the experimental uncertainties that can be significant at times.
- Uncertainty Quantification (UQ): Rigorous UQ has not yet been applied to engine CFD simulations to understand the relative importance of uncertainties from experimental boundary conditions vs. chemical kinetics vs. sub-model constants

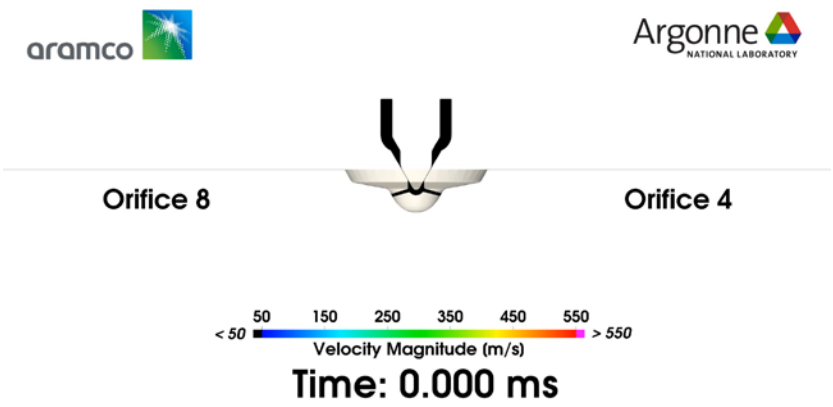
PROPOSED FUTURE WORK

1) Extend the *one-way coupling* approach and couple with the new TFM combustion solver to predict the influence of nozzle flow on combustion and emissions
2) CRADA project with Cummins and CSI (FY16-FY18)
   - Continue improving the cavitation erosion modeling framework by integrating material properties into the erosion criteria and perform more quantitative validation
   - Development of fluid structure interaction model to predict needle transients: validation against x-ray measurements of needle lift and wobble
   - Develop "engineering best-practices" to enable industry use the "real-geometry" from injectors
3) Validate LTP ignition models and continue the evaluation of LTP post-discharge characteristics on ignition processes at engine relevant conditions.
4) Continue working towards one single comprehensive ignition model consisting of a library of sub-models based on the ignition system of interest.

5) Future validation of the TFM with ANN approach for multi-component diesel surrogates developed at LLNL:
   - Constant volume chamber data from Sandia to improve predictions of ignition delay and flame LOL (in collaboration with L. Pickett)
   - Optical engine data from Sandia (in collaboration with C. Mueller)
   - Understand and report run-time vs. accuracy trade-off of turbulence models and detailed kinetic mechanisms

SUMMARY

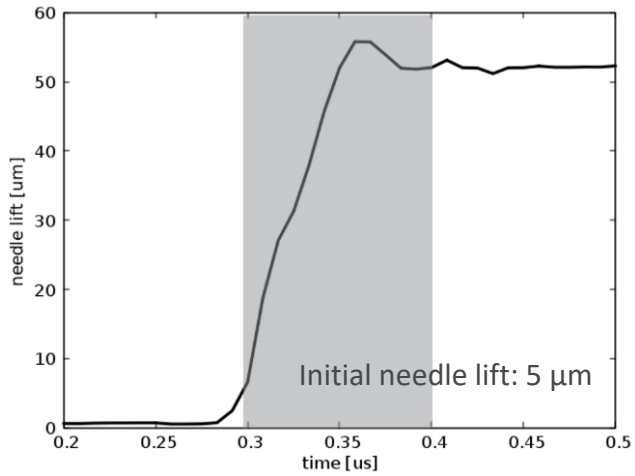
- **Objective**
  - Development of predictive spray, turbulence, ignition, and combustion models aided by HPC tools and comprehensive validation.
- **Approach**
  - Coupling expertise from DOE Office of Science on fundamental chemical kinetics, industrial partners, and HPC resources for development of robust engine models.
- **Collaborations and coordination**
  - With industry, academia, and national laboratories; through ECN with researchers world-wide.
  - Through VERIFI collaborations with light-duty, heavy-duty, software vendors, and energy companies.
- **Technical Accomplishments**
  - A new cavitation erosion model developed and implemented for further testing.
  - Real geometry results in faster spray breakup and lower SMDs compared to a nominal geometry.
  - One way coupling approach shown in AMR2017 has been applied for diesel injectors and can uniquely capture the effect of nozzle flow on fuel spray.
  - Full coupled ELSA model implemented and validated for a multi-hole injector.



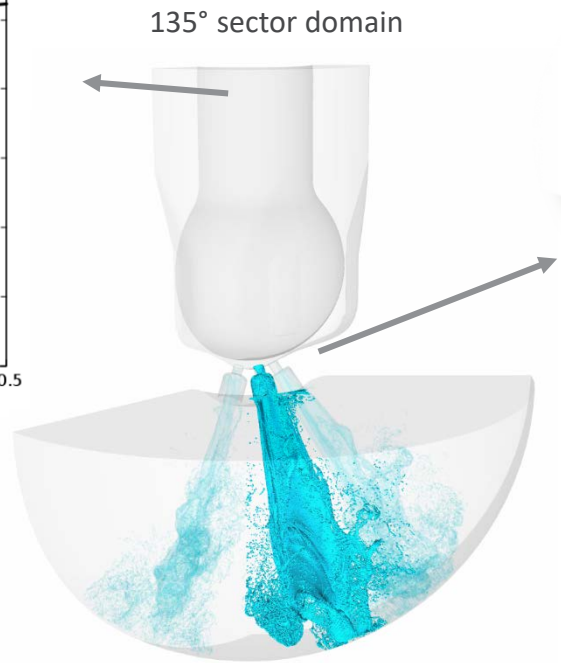
  - Use of ML tools (Artificial Neural Network) further enabled the implementation of full chemistry (without mechanism reduction) in engine simulations.
  - LTP modeling improved and quantitatively validated against experiments.
  - Ignition simulated with a CFD engine code using realistic energy/species deposition from LTP modeling.

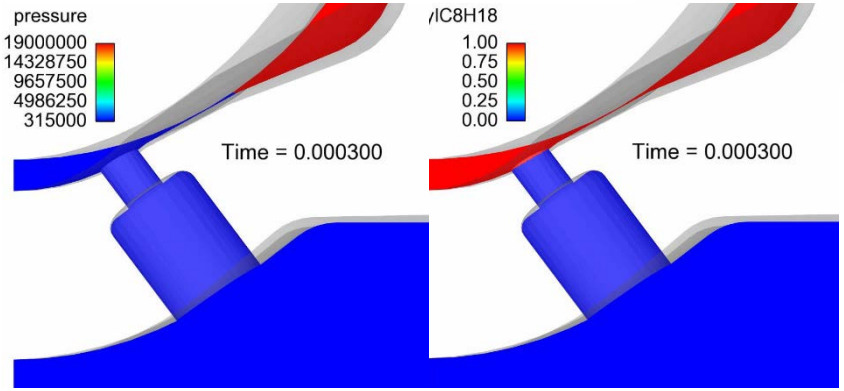
Technical Back-Up Slides

REAL GEOMETRY SIMULATION SET-UP DETAILS



Needle lift profile





Pressure Species

Initialization of computational domain

	Pressure	Species
Chamber	3.15 bar	N2
Orifice	3.15 bar	N2
Sac (below min. gap)	3.15 bar	Iso-octane
Sac (above min. gap)	190 bar	Iso-octane

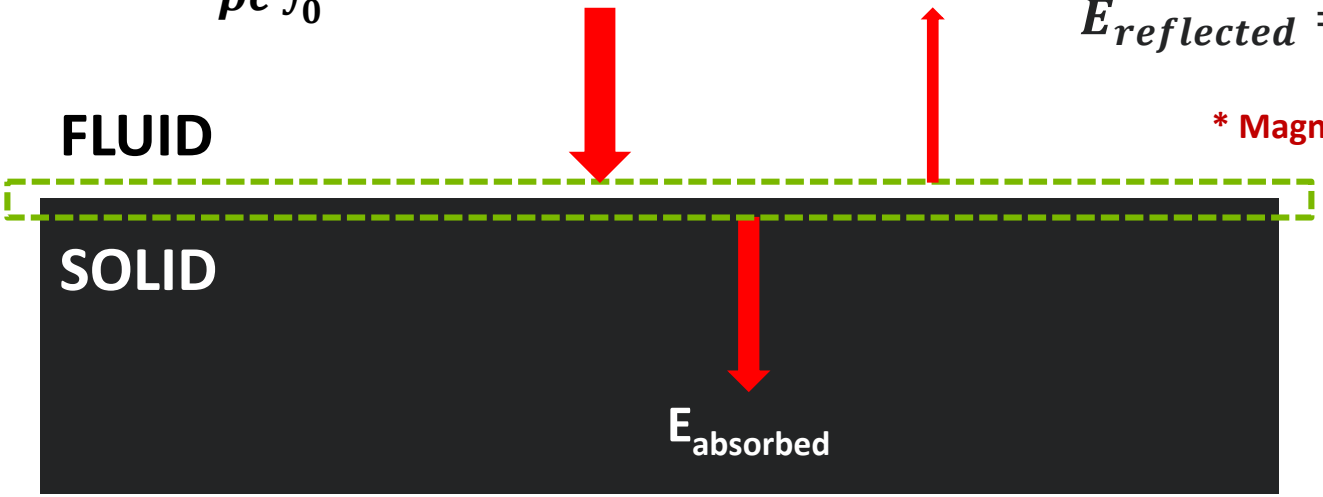
NEW CAVITATION EROSION MODEL DEVELOPMENT*

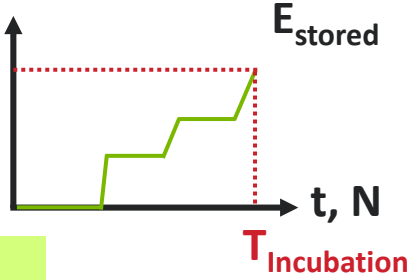
$$E_{impact,i} = \frac{\mathcal{A}}{\rho c}\int_0^{\tau} p^2(t)dt$$

$$E_{reflected} = E_{impact}\ (P < \sigma_Y)$$

$$E_{reflected} = 0\ (P > \sigma_Y)$$

* Magnotti, Som et al., ICLASS 2018



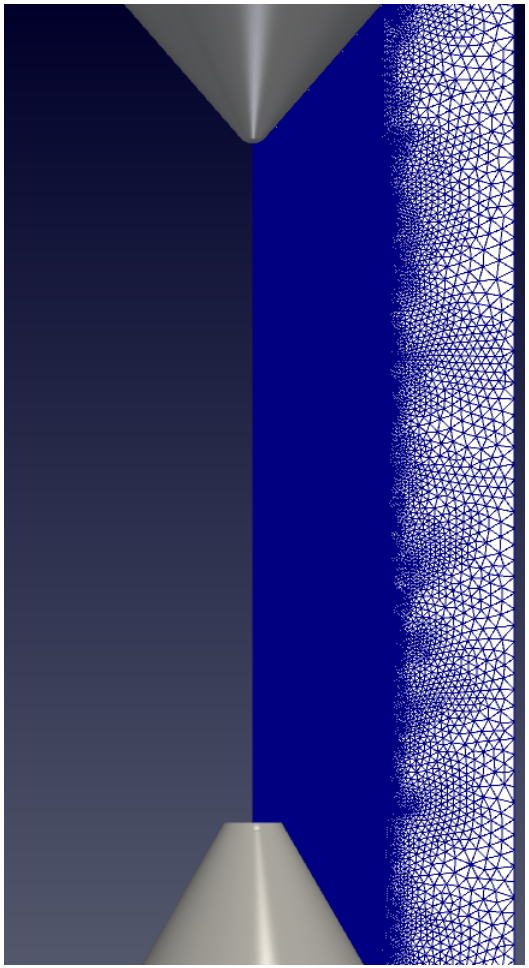


$$E_{stored}(N) = \sum_{i=1}^{N} E_{impact,i} = \sum_{i=1}^{N} \frac{\mathcal{A}}{\rho_l c_l}\int_0^{\tau} p^2(t)dt$$

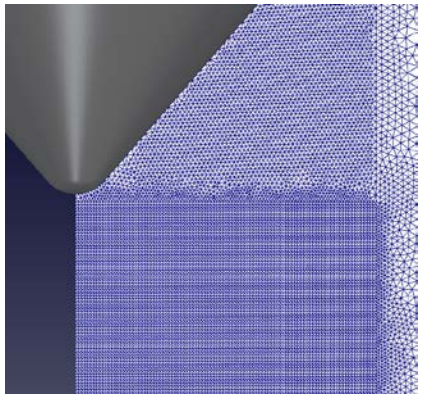
- Material failure would be predicted when E_{stored} exceeds a critical threshold. However, determination of the critical energy threshold for material rupture is not straightforward.
- Within the incubation period, a multitude of cavitation cloud collapse events with varying strain rates can be expected to occur.
- In the current stage of this work, a critical energy is not yet defined, but is deemed as an important parameter to be characterized in future investigations.
- In its current form, E_{stored} is used as a qualitative measure of cavitation erosion. However, based on its ability to capture the effect of repeated impacts on the material state and current progress within the incubation period, the newly derived E_{stored} provides an improved characterization of cavitation erosion over existing metrics in the literature.

NON-EQUILIBRIUM PLASMA MODELING

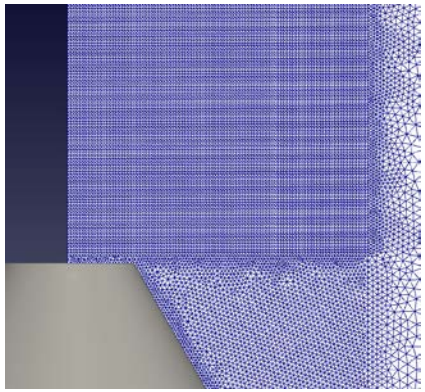
Simulation Setup (VIZGLOW)



Anode details



Cathode details



Plasma model highlights

- 2-D axis-symmetric domain
- O_2-N_2 plasma chemistry for high pressure applications with 18 species: E, O_2, O_2*, O_2a1, O_2b1, O_2+, O_2-, O, O-, O_4+, O_2+N_2, N_2, N_2a1, N_2A, N_2B, N_2C, N_2+, N_4+
- Photoionization and bulk energy are modeled

Boundary and initial conditions

- 5.2 mm gap between electrodes
- Rounded Anode tip (measured)
- Flat Cathode tip (measured)
- Mixture: 20.95% O_2, 79.05% N_2 (%vol.)
- T = 343K, several pressure values
- Voltage provided by experiments

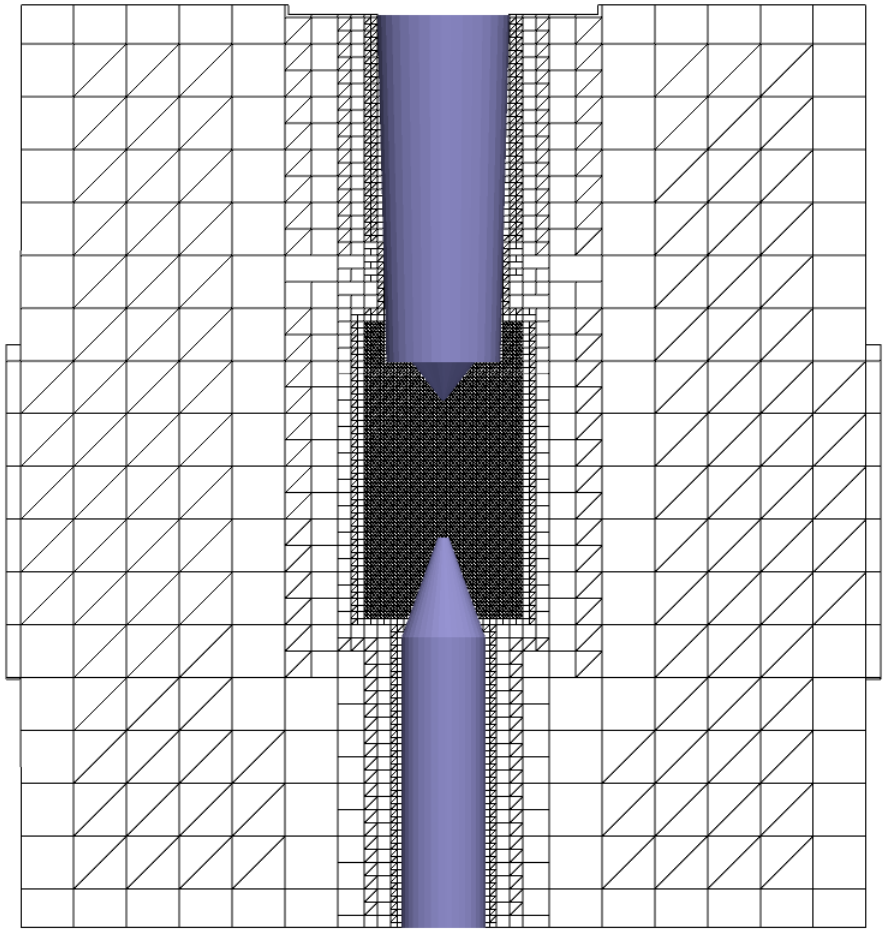
Mesh configuration

- Mixed quad/tri mesh with 10 µm min size
- Uniform quad cells in the center gap
- Total cell count 80,000

We evaluated the effect of mesh size as well as typical model uncertainties, namely the initial Electron seeding, geometry irregularities, Electron cross section (through collision frequency)

LTP IGNITION SIMULATION DETAILS

Simulation Setup (CONVERGE)



Calorimetry detailed geometry from Isaac Ekoto (ACS006)

Assumptions

- Discharge in air/fuel mixture identical to the 100% air case (realistic)
- Discharge does not change from pulse to pulse (not realistic)

Ignition/Combustion model highlights

- Full 3-D domain of Sandia calorimetry
- RANS (k-ε)
- SAGE solver (direct chemistry)
- C_8H_{18} 110 species, 488 reactions (reduced from full-size LLNL mechanism)

Boundary and initial conditions

- 5.2 mm gap between electrodes
- Rounded Anode tip (measured)
- Flat Cathode tip (measured)
- T = 343K, p = 1.5 bar, ϕ = 1.0

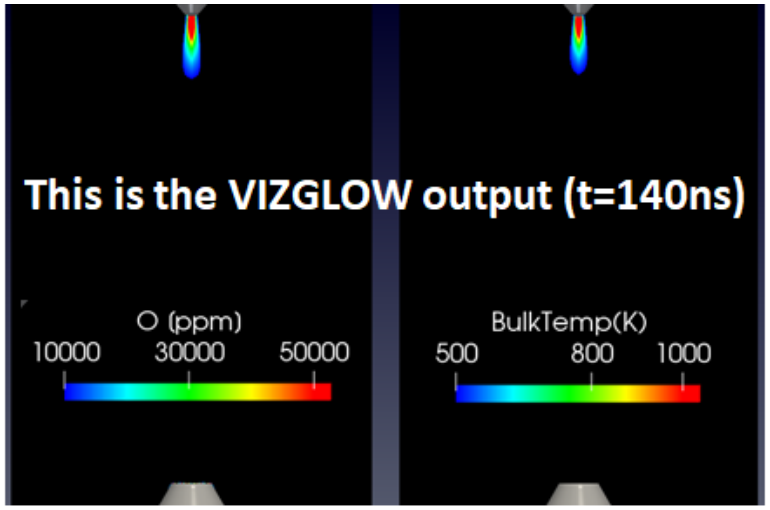
Mesh configuration

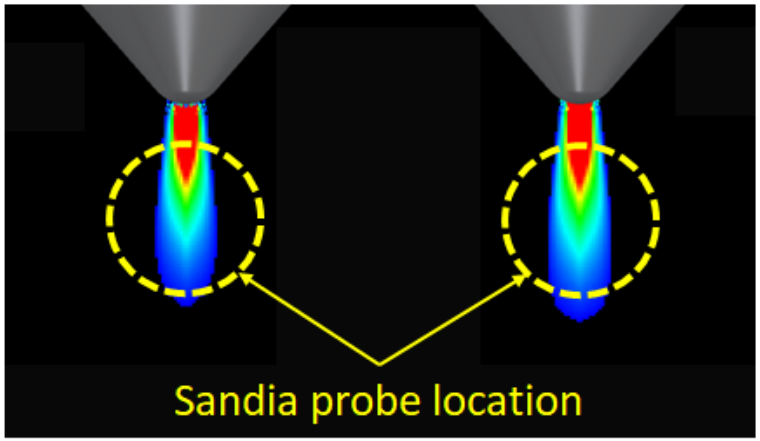
- Base 2.0 mm, AMR 0.25 mm, Embedding 0.125 mm (typical engine resolution)
- Total cell count = 200-600k

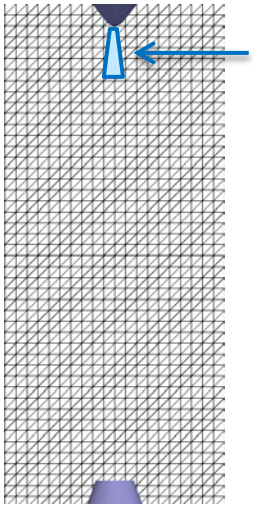
Mesh size and turbulence model are not optimized. The goal was to demonstrate that combustion can be initiated and sustained by LTP. Proper experimental dataset is needed for validation.

LTP IGNITION SIMULATION DETAILS

LTP deposition (from VIZGLOW to CONVERGE)



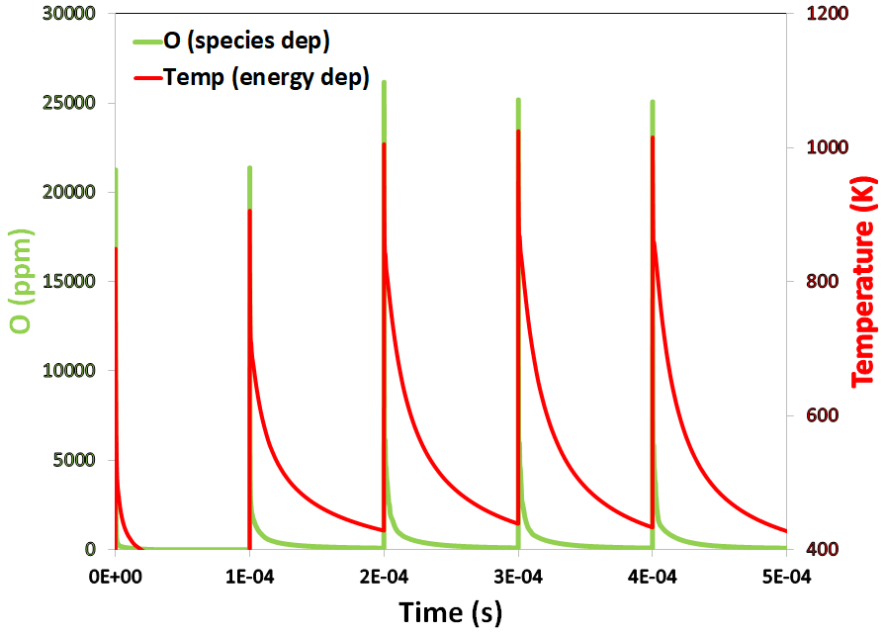




Deposition of thermal energy and O at each pulse time (100 ms).

The duration of the deposition in CONVERGE is 100 ns, as typical plasma discharge duration

The time-step of the CONVERGE simulation is forced to be 10 ns (10^{-8} s) to fully resolve the mixed Energy/species deposition



The imposed deposition delivers the same quantities (O and Temp) measured at Sandia